201-14713

Crompton

Product Safety and Regulatory Affairs

August 27, 2003

Marianne L. Horinko
Acting Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Attn: Chemical Right-To-Know Program

Dear Administrator Horinko,

Crompton Corporation is submitting the enclosed Robust Summary and Test plan for the following chemical:

2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propane-1,3-diyl bis[3-(dodecylthio) propionate (CAS # 29598-76-3).

If you have any questions, please contact me at 203-573-3390 or e-mail to mark_thomson@cromptoncorp.com

Sincerely,

Dr. Mark A. Thomson
Manager, Toxicology & International Product Registration
Crompton Corporation
Middlebury, CT 06749
USA

201-14713A

HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

Propionic acid, 3-(dodecylthio)-, neopentanetetrayl ester

CAS No. 29598-76-3

Submitted to the US EPA

BY

Crompton Corporation.

Table of Contents

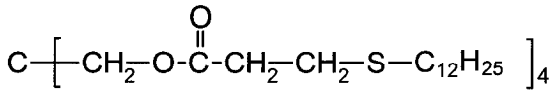
Test Plan for Propionic acid, 3-(dodecylthio)-, neopentanetetrayl ester

1. General Information

1.1 CAS Number: 29598-76-3

1.2 Molecular Weight: 1161.95

1.3 Structure and formula: $C_{65}H_{124}O_8S_4$



1.4 Introduction

Propionic acid, 3-(dodecylthio)-, neopentanetetrayl ester is an antioxidant for use with polyolefins (particularly polyethylene and polypropylene) and engineering thermoplastics.

2. Review of Existing Data and Development of Test Plan

Crompton Corporation has undertaken a comprehensive evaluation of all relevant data on the SIDS endpoints of concern for propionic acid, 3-(dodecylthio)-, neopentanetetrayl ester.

The availability of the data on the specific SIDS endpoints is summarized in Table 1. Table 1 also shows data gaps that will be filled by additional testing.

Table 1: Available adequate data and proposed testing on Propionic acid, 3-(dodecylthio)-, neopentanetetrayl ester

CAS No. 10081-67-1	Information Available?	GLP	OECD Study?	Other Study?	Estimation Method?	Acceptable?	SIDS Testing required?
	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
Physicochemical							
Melting Point	Y	N				Y	N
Boiling Point	Y	N				Y	N
Vapour Pressure	Y	N			Y	Y	N
Water Solubility	Y	N			Y	Y	N
Partition Coefficient (Kow)	Y	N			Y	Y	N
Environmental Fate							
Biodegradation	Y				Y	Y	N
Hydrolysis	Y				Y	Y	N
Photodegradation	Y				Y	Y	N
Transport and Distribution between Environmental Compartments	Y				Y	Y	N
Ecotoxicology							
Acute Fish	Y				Y	Y	N
Acute Daphnia	Y				Y	Y	N
Acute Algae	Y				Y	Y	N
Toxicology							
Acute Oral	Y					Y	N
Repeat Dose toxicity	N						Y
Genetic toxicity – Gene mutation	Y					N	Y
Genetic toxicity – Chromosome aberration	N						Y
Reproductive toxicity	N						Y
Developmental toxicity/teratogenicity	N						Y

A. Evaluation of Existing Physicochemical Data and Proposed Testing

1. Melting Point

The Safety Data Sheet for the chemical quotes a melting point of 50-51°C.

2. Boiling Point

The Safety Data Sheet for the chemical reports that the substance decomposes before boiling.

3. Vapour Pressure

The vapour pressure is estimated to be $9x10^{-24}$ hPa at 25°C using MPBPWIN v1.40.

4. Water Solubility

The water solubility is estimated to be $1.268x10^{-21}$ mg/L using WSKOW v1.40.

5. Partition Coefficient

The partition coefficient is estimated as log Kow = 24.77 using KOWWIN v1.66. Because of the very high estimated value, which is due to the very low water solubility, it is considered unnecessary to derive a value for log Kow experimentally.

Summary of Physicochemical Properties Testing: Existing data for melting point, boiling point, vapour pressure, water solubility and partition coefficient are considered to fill these endpoints adequately.

B. Evaluation of Existing Environmental Fate Data and Proposed Testing

1. Biodegradation

The biodegradability of the chemical has been estimated using Biowin v4.00 and the results indicate the chemical to be readily biodegradable.

2. Hydrolysis

The half life at pH 7 is estimated to be greater than one year using HYDROWIN v1.67. It is not practicable to measure the hydrolysis for a substance with such low water solubility.

3. Photodegradation

The potential for photodegradation has been estimated using the AOPWIN v1.90, and indicates atmospheric oxidation via OH radicals reaction with a half-life of 0.9 hours.

4. Transport and Distribution between Environmental Compartments

An Epiwin Level III Fugacity Model calculation has been conducted for the chemical and indicates distribution mainly to sediment for emissions of 1000 kg/hr simultaneously to air water and soil compartments.

Summary of Environmental Fate Testing: The endpoints for biodegradation, hydrolysis, photodegradation and transport and distribution between environmental compartments are filled adequately.

C. Evaluation of Existing Ecotoxicity Data and Proposed Testing

1. Acute Toxicity to Fish

The LC50 (96 h) is estimated to be $1.16x10^{-10}$ mg/L using ECOSAR v0.99g. This is higher than the estimated solubility of the chemical.

2. Acute Toxicity to Algae

The EC50 (96 h) is estimated to be $2.13x10^{-11}$ mg/L, using ECOSAR v0.99g. This is higher than the estimated solubility of the chemical.

3. Acute Toxicity to Daphnia

The EC50 (48 h) is estimated to be $1.76x10^{-18}$ mg/L using ECOSAR v0.99g. This is higher than the estimated solubility of the chemical.

Summary of Ecotoxicity Testing: Toxicity to aquatic species is estimated to occur at a level higher than the estimated solubility of the chemical. The chemical is predicted not to be acutely toxic to aquatic organisms and the endpoints are considered to be filled adequately.

C. Evaluation of Existing Human Health Effects Data and Proposed Testing

1. Acute Oral Toxicity

The LD50 (rat) is reported as >15000 mg/kg b.w. in the safety data sheet for this chemical. Although there is insufficient information to assess the reliability of this reported value, it is considered to be unnecessary to perform a new study as the range finding study to select doses for the OECD 422 study will be used to provide further indication of acute oral effects.

2. Repeat Dose Toxicity

The repeat dose toxicity of will be determined using OECD Method 422.

3. Genotoxicity

The safety data sheet for this chemical reports that it tested negative in an Ames test, however there is insufficient information to assess the reliability of the result. An Ames test will be conducted using OECD 471.

An in vitro chromosome aberration study will be conducted using OECD Method 473.

4. Reproductive and Developmental Toxicity

The developmental and reproductive toxicity in rat will be determined using OECD Method 422.

Summary of Human Health Effects Testing: The repeat dose toxicity combined with the developmental and reproductive toxicity will be evaluated using OECD Method 422. The potential to cause in vitro chromosomal aberrations will be determined using OECD Method 473 and an Ames test will be performed using OECD Method 471. The existing data for acute oral toxicity, when combined with the range finding data from the OECD 422 study is considered to fill this endpoint adequately.

3. Evaluation of Data for Quality and Acceptability

The collected data were reviewed for quality and acceptability following the general US EPA guidance [2] and the systematic approach described by Klimisch et al [3]. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to ecotoxicology and human health endpoint studies per EPA recommendation [4]. The codification described by Klimisch specifies four categories of reliability for describing data adequacy. These are:

(1) Reliable without restriction: Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.

(2) Reliable with Restrictions: Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.

(3) Not Reliable: Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

(4) Not Assignable: Includes studies or data in which insufficient detail is reported to assign a rating, e.g. listed in abstracts or secondary literature.

4. References

[1] US EPA, EPI Suite Software, 2000

[2] USEPA (1998). Guidance for Meeting the SIDS Requirements (The SIDS Guide). Guidance for the HPV Challenge Program. Dated 11/2/98.

[3] Klimisch, H.-J., et al (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5

[4] USEPA (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 2/10/99.

201-14713B

I U C L I D

Data Set

Robust Summaries

Existing Chemical	:	ID: 29598-76-3
Memo	:	Crompton US HPV
CAS No.	:	29598-76-3
EINECS Name	:	2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propane-1,3-diyl bis[3-(dodecylthio)propionate]
EC No.	:	249-720-9
Molecular Formula	:	C65H124O8S4
Status	:	
Memo	:	Crompton Corporation US HPV Seenox 412S
Printing date	:	26.06.2003
Revision date	:	
Date of last update	:	26.06.2003
Number of pages	:	1

2.1 MELTING POINT

Value	:	50 - 51 °C
Sublimation	:	
Method	:	other: no data
Year	:	2002
GLP	:	no data
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Reliability	:	(2) valid with restrictions

28.03.2003 (1)

2.2 BOILING POINT

Decomposition	:	yes
Method	:	other: no data
Year	:	2002
GLP	:	no data
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Reliability	:	(2) valid with restrictions

28.03.2003 (1)

2.4 VAPOUR PRESSURE

Value	:	9E-24 hPa at °C
Decomposition	:	
Method	:	other (calculated): MPBPWIN v1.40
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Method	:	Physical property inputs: Melting Point = 50 °C (experimental) Boiling Point = 1065.96 °C (estimated using MPBPWIN v1.40)
Reliability	:	(2) valid with restrictions

28.03.2003 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	24.77 at °C
pH value	:	
Method	:	other (calculated): KOWWIN v1.66
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Reliability	:	(2) valid with restrictions

24.01.2003 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	1.268E-21 mg/L at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: Estimated using WSKOW v1.40
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Method	:	Inputs: Log Kow = 24.77 (estimated) Melting Point = 50 °C (experimental)
Reliability	:	(2) valid with restrictions

24.01.2003 (2)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	.9 hour(s)
Degradation	:	% after
Quantum yield	:	
Deg. product	:	
Method	:	other (calculated): AOPWIN v1.90
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Test condition	:	12 hr day, 1.5E6 OH/cm3
Reliability	:	(2) valid with restrictions

28.03.2003 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	> 1 year at °C
t1/2 pH9	:	at °C
t1/2 pH 8	:	59.4 day(s) at °C
Deg. product	:	
Method	:	other (calculated):HYDROWIN v1.67
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Reliability	:	(2) valid with restrictions

28.03.2003 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: EPIWIN Level III Fugacity Model
Year	:	2002
Test condition	:	Henry's Law Constant: 6.9E-17 atm-m3/mole (Henrywin program) Vapor pressure: 6.81E-24 mmHg (Mpbpwin program) Log Kow: 24.8 (Kowwin program) Soil Koc: 2.41E+24 (calc by model) Melting point: 50 °C (experimental)

1000 kg/hr emissions to air, water and soil compartments.

Test substance : Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate]
CAS #: 29598-76-3

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	0.0306	1.79	1000
Water	2.38	1440	1000
Soil	28.9	1440	1000
Sediment	68.7	5760	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	6.58E-30	906	23.4	30.2	0.78
Water	1.26E-41	87.7	182	2.92	6.07
Soil	1.15E-43	1060	0	35.4	0
Sediment	1.23E-41	632	105	21.1	3.5

Persistence time: 2550 hr
Reaction time: 2840 hr
Advection time: 24600 hr
Percent reacted: 89.6
Percent advected: 10.4

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):
Air: 1.79
Water: 1440
Soil: 1440
Sediment: 5760
Biowin estimate: 2.173 (months)

Advection times (hr):
Air: 100
Water: 1000
Sediment: 5E+4

Reliability : (2) valid with restrictions
28.03.2003 (2)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Deg. product :
Method : other: Estimation using BIOWIN v4.00
Year : 2003
GLP :
Test substance : Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate]
CAS #: 29598-76-3

Result : MITI Linear Biodegradation Probability: 1.467
MITI Non-linear Biodegradation Probability: 0.964

The substance is predicted to be readily biodegradable

Reliability : (2) valid with restrictions
28.03.2003 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Method	:	other: Estimation using ECOSAR v0.99g
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Result	:	Predicted LC50 (96 h) = 1.16E-10 mg/L. This is higher than the predicted solubility of the chemical.
Test condition	:	Inputs: Log Kow = 24.77 (Kowwin estimate) Melting point = 50 °C (experimental) Water solubility 1.14E-19 mg/L (calculated by program)
Reliability	:	(2) valid with restrictions

28.03.2003 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Method	:	other: Estimation using ECOSAR v0.99g
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Result	:	Predicted LC50 (48 h) = 1.76E-18 mg/L. This is higher than the predicted solubility of the chemical.
Test condition	:	Inputs: Log Kow = 24.77 (Kowwin estimate) Melting point = 50 °C (experimental) Water solubility 1.14E-19 mg/L (calculated by program)
Reliability	:	(2) valid with restrictions

28.03.2003 (2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
Method	:	other: Estimation using ECOSAR v0.99g
Year	:	2002
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3

Result	:	Predicted EC50 (96 h) = 2.13E-11 mg/L. This is higher than the predicted solubility of the chemical.
Test condition	:	Inputs: Log Kow = 24.77 (Kowwin estimate) Melting point = 50 °C (experimental) Water solubility 1.14E-19 mg/L (calculated by program)
Reliability 28.03.2003	:	(2) valid with restrictions (2)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 15000 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Reliability	:	(4) not assignable

28.01.2003 (1)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	negative
Method	:	
Year	:	
GLP	:	
Test substance	:	Chemical name: 2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]propan-1,3-diylbis[3-(dodecylthio)propionate] CAS #: 29598-76-3
Reliability	:	(4) not assignable

28.01.2003 (1)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Crompton Corporation, Seenox 412S Safety Data Sheet, Rev. 1.2, February 2002

(2) US EPA, EPIWIN v3.10, EPI Suite Software, 2000